

The austenitic peak stress model of low alloy steel at elevated temperature based on the valence electron theory

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ABSTRACT

Firstly the average coefficient of thermal expansion of the low alloy steel was calculated with JmatPro software, then the lattice constants both of no carbon-containing and carbon-containing austenite unit cells are computed at high temperature with the weighted average method. The Austenitic valence electron parameters and their statistical values are calculated based on above lattice constants using the empirical electron theory.

The austenitic unit cells in this paper include no carbon-containing, carbon-containing, silicon-containing, manganese-containing and molybdenum-containing. Then their binding energies were calculated. Finally using the sum of both the binding energy based on the valence electron statistic parameters and the mole fractions of the above elements in low alloy steel, the semi-empirical model of austenitic peak stress at high-temperature was established, by combining with Medina's austenitic measurement data. By the fitted regression relationship of binding energy with the iron, carbon, silicon, manganese and molybdenum elements in the low alloy steel, the austenite peak stresses simplified empirical model was obtained. The results show that: the austenitic peak stress model presented in this paper was provided with good precision, indicating that the establishment method of peak stress model of austenite at high temperature based on statistical parameters' binding energy is valid. Since considering the impact of more additional chemical elements in the low alloy steel the empirical model provides an effective way for low alloy steel deformation resistance calculation.

Keywords: Valence electron theory, Binding energy, Austenite at high-temperature, Peak stress

1. INTRODUCTION

The low alloy steel is the most widely used steel, while the hot forming is its main production method. The low alloy steel under hot forming at a high temperature is in austenitic state, so that the calculation of the austenite strength at elevated temperature is particularly important for its hot forming. So far, the most of calculations are based on empirical methods^[1-6].

The low alloy steel belongs to the polyatomic system. Today it has still been very difficult to establish the polyatomic system interaction potential. And it will be difficult to calculate the phase lattice parameter with different chemical composition in the low alloy steel, therefore the phase electrical parameters required in this paper to be calculated can not be given by Schrödinger equation. In the alloy strength calculation, Liu has carried out a lot of researches, such as the methods to use the alloy phase the strongest bond valence electrons number n_A , and the minimum electron density difference $\Delta\rho$ at the phase

interface to express the strength, however, all works mentioned above have been limited at room temperature^[7-11]. Although the high temperature phase valence electron parameters have been studied, but those did not use to solve the alloys strength^[12,13].

The work in this paper inspired by Liu's works^[7-10], is going to establish austenite peak stress model at the high temperature using the binding energy of austenitic phase in the low alloy steel. Firstly the lattice constant of austenite at high temperature is calculated, and then the statistical value of its covalent valence electrons and the binding energy are calculated, finally the peak stress model based on the measured data of MEDINA^[5] is established.

2. THE AUSTENITIC LATTICE CONSTANT AT HIGH TEMPERATURE

Using JmatPro software the austenitic thermal expansion coefficient with different chemical

composition of the low alloy steel was calculated, further the fitting equation of the expansion coefficient was gained (Table 1).

According to the austenite lattice constant relationship with the carbon content of Ref. [14], the linear regression equation was gained in Figure 1.

$$a = 3.55733 + 0.00987C(\text{at}\%)$$

To convert the mass percentage from the atomic percentage, the equation becomes

$$a = 3.55904 + 0.04249C(\text{wt}\%)$$

Table 1: Chemical composition(wt%), grain size D and thermal expansion coefficient equations

Steel No	C	Si	Mn	Mo	D (μm)	thermal expansion coefficient equations $a(T) (^{\circ}\text{C})(\times 10^{-6})$
Fe	≤ 0.003	0	0	0		$-26.41 + 6.27 \ln(T - 482.12)$
C1	0.15	0.21	0.74	0	187	$-24.66 + 6.08 \ln(T - 485.59)$
C2	0.36	0.2	0.82	0	189	$-21.08 + 5.59 \ln(T - 473.00)$
C3	0.53	0.21	0.71	0	179	$-18.04 + 5.18 \ln(T - 466.35)$
SI	0.11	0.26	0.55	0	143	$-25.21 + 6.15 \ln(T - 490.77)$
S2	0.11	1.65	0.47	0	104	$-24.79 + 6.21 \ln(T - 492.75)$
MI	0.11	0.26	0.68	0	212	$-25.20 + 6.15 \ln(T - 489.89)$
M2	0.11	0.25	1.55	0	192	$-25.56 + 6.23 \ln(T - 479.50)$
Mo1	0.44	0.24	0.79	0.26	180	$-19.70 + 5.41 \ln(T - 469.85)$
Mo2	0.44	0.23	0.79	0.38	205	$-19.81 + 5.42 \ln(T - 469.87)$
Mo3	0.42	0.27	0.79	0.18	193	$-20.05 + 5.46 \ln(T - 469.88)$

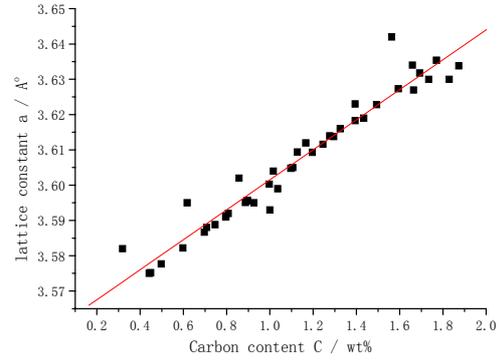


Figure 1 Relationship between the lattice constant and carbon content

The no carbon-containing austenitic lattice constant at high temperature is

$$a_0(T) = a_0 \{1 + \alpha(T)(T - 25)\}$$

Where, a_0 is no carbon-containing unit cell lattice constant at 25°C.

The austenitic lattice constant in the low alloy steel at high temperature is

$$a(T) = a \{1 + \alpha(T)(T - 25)\}$$

Since the lattice constant of the carbon-containing unit cell $a_c(T)$ can not be measured directly from the experiment, it can only be obtained based on the weighted average method of the mix austenite lattice constant $a(T)$ with different carbon content^[15]. Let A_c be carbon atomic percentage, and $a_0(T)$ be no carbon-containing unit cell lattice constant, then

$$a_c(T) = \frac{1}{4} \left(5 - \frac{100}{A_c}\right) a_0(T) + \frac{1}{4} \left(\frac{100}{A_c} - 1\right) a(T)$$

Thus, according to these lattice constants, the lattice experimental bond distance $D(na) = f(a_0(T))$ or $f(a_c(T))$ of the unit cell of no carbon-containing, carbon-containing, silicon-containing, manganese-containing and molybdenum-containing can be calculated, then the covalent bond electron number nA , nB and the lattice electron number nI can be calculated using the empirical electron theory, and finally their statistical values of nA , nB and nI are carried out.

3. THE AUSTENITIC BINDING ENERGY AT HIGH TEMPERATURE

With the empirical electron theory to characterize the alloy properties, it often needs to identify the single most probable configuration from $10^4 \sim 10^8$

configurations, which would be quite difficult. According to the idea that macroscopic physical quantity should be the expression of the microscopic physical state, the statistic value of n_A , n_B and n_l in this paper will be used to calculate the austenite binding energy at high temperature.

The statistical value of the electron structure parameters is as follows

$$n'_a = \sum_{i=1}^{\sigma_N} n_{ai} C_i \quad \text{and} \quad n'_l = \sum_{i=1}^{\sigma_N} n_{li} C_i$$

Where, n_{ai} is the number of electrons in a covalent bond on any one atomic configuration of all cell configurations, n_{li} is the lattice electron number on any one atomic configuration, C_i is the probability of atomic configuration, $C_i = 1/\sigma_N$, σ_N is the configuration number.

In this paper, the statistical the number n'_A of covalent electrons on the strongest bond, the covalent electrons n'_B on the second strong bond, and statistics lattice electrons n'_l will be calculated. Then according to Yu Ruihuang's binding energy formula^[16]

$$E_C = b \left\{ \sum_a \frac{I_a n_a}{D_{(n_a)}} f + \frac{n_l}{D} f' + am^{3d} - CW \right\}$$

Where, I_a is equivalent bond number, m^{3d} is magnetic electrons

number, $W = \frac{n_d C_{h11} + n'_d C_{t11} + m^{3d}}{z}$, (n_d and n'_d

are head h and tail t dummy electrons number, z is the total electron number of atomic shell).

In accordance with rank 11 of Fe B-type hybrid in austenite,

$b = 37.5 \text{ kJ/mol}$, $f = 1.9368$, $f' = 0.7067$, $a = 0.1542$, $m^{3d} = 1.998$, $C = 2.7210$, $W = 0.3333$, it can be obtained,

$$E'_C = 157 \left\{ 1.9368 \left(\frac{I_A n_A}{D_{(n_A)}} + \frac{I_B n_B}{D_{(n_B)}} \right) + 0.7067 \frac{n_l (I_A + I_B)}{I_A D_{(n_A)} + I_B D_{(n_B)}} + 0.3081 - 0.9069 \right\} \quad (3)$$

Then, the unit cell binding energy with statistical values becomes

$$\bar{E} = 157 \left\{ 1.9368 \left(\frac{I_A n'_A}{D_{(n_A)}} + \frac{I_B n'_B}{D_{(n_B)}} \right) + 0.7067 \frac{n'_l (I_A + I_B)}{I_A D_{(n_A)} + I_B D_{(n_B)}} + 0.3081 - 0.9069 \right\}$$

Let the mole fraction of carbon, manganese, silicon, molybdenum, and iron element in low alloy steel be as follows

$$\begin{aligned} x_C &= (C/12)/(C/12+Mn/55+Si/32+Mo/96+(100-C-Mn-Si-Mo)/56) \\ x_{Mn} &= (Mn/55)/(C/12+Mn/55+Si/32+Mo/96+(100-C-Mn-Si-Mo)/56) \\ x_{Si} &= (Si/32)/(C/12+Mn/55+Si/32+Mo/96+(100-C-Mn-Si-Mo)/56) \\ x_{Mo} &= (Mo/96)/(C/12+Mn/55+Si/32+Mo/96+(100-C-Mn-Si-Mo)/56) \\ x_{Fe} &= ((100-C-Mn-Si-Mo)/56)/(C/12+Mn/55+Si/32+Mo/96+(100-C-Mn-Si-Mo)/56) \end{aligned}$$

Where, C, Mn, Si and Mo are in the mass percentage.

In accordance with the weighted average method, the total binding energy becomes

$$E = x_{Fe} \bar{E}_{\gamma Fe} + x_C \bar{E}_{\gamma FeC} + x_{Mn} \bar{E}_{\gamma FeMn} + x_{Si} \bar{E}_{\gamma FeSi} + x_{Mo} \bar{E}_{\gamma FeMo}$$

The relationship between the total binding energy and the chemical elements by nonlinear fitting method is as follows

$$E = 2.2561C - 1.8927Mn - 3.3162Si - 0.7632Mo + 1159.0327(T + 273)^{-0.1335} \quad (1)$$

The fitting correlation coefficient is 0.9980.

3. PEAK STRESS MODEL OF HIGH-TEMPERATURE AUSTENITE

According to the hall-petch formula and Misaka formula^[17] the peak stress model was established.

$$\sigma_p = (s_0 + \frac{s_0}{\sqrt{D}}) \dot{\epsilon}^m \exp\left(\frac{p_1 E^{p_2}}{T + 273}\right) \quad (2)$$

Where, D is the grain size (μm), T is the temperature ($^{\circ}\text{C}$), $\dot{\epsilon}$ is strain rate (1/s), s_0 , m , p_1 , and p_2 are undetermined parameters.

According to Menina high temperature austenitic peak stress measured data^[5], the model is fitted as follows

$$\sigma_p = \left(3.2426 + \frac{3.2426}{\sqrt{D}} \right) \dot{\epsilon}^{0.1193} \exp\left(\frac{2107890E^{-1.0069}}{T + 273}\right) \quad (3)$$

The correlation coefficient fitted is 0.9460.

For the austenite of low alloy steel at high temperature including carbon, silicon, manganese and chromium elements the total binding energy in equation (3) can be substituted by the formula (1).

The comparison of the peak stress models is shown in Figure 2. Our model's variance is 64.0404, while Medina model's variance is 66.1120. The standard deviation in our model is 8.0025, while the standard deviation at Medina model is 8.1309, so our model is more accurate.

Table 2 The binding energy in various kinds of steel (kJ/mol)

Steel No	$T(^\circ\text{C})$	$\bar{E}_{\gamma\text{Fe}}$	$\bar{E}_{\gamma\text{FeC}}$	$\bar{E}_{\gamma\text{FeSi}}$	$\bar{E}_{\gamma\text{FeMn}}$	$\bar{E}_{\gamma\text{FeMo}}$	E
Cl	900	450.96	501.67	281.68	276.70		449.39
	1000	446.49	494.52	276.75	272.85		444.90
	1100	441.65	488.20	271.25	269.52		440.07
C2	900	450.96	499.06	281.68	276.70		449.74
	1000	446.49	494.08	276.75	272.85		445.26
	1100	441.65	489.30	271.25	269.52		440.44
C3	900	450.96	499.56	281.68	276.70		450.30
	1000	446.49	495.47	276.75	272.85		445.83
	1100	441.65	490.55	271.25	269.52		441.01
SI	900	450.96	505.42	281.68	276.70		449.51
	1000	446.49	498.50	276.75	272.85		445.02
	1100	441.65	489.60	271.25	269.52		440.17
S2	900	450.96	439.55	281.68	276.70		445.28
	1000	446.49	418.33	276.75	272.85		440.71
	1100	441.65	409.24	271.25	269.52		435.84
MI	900	450.96	502.63	281.68	276.70		449.26
	1000	446.49	494.22	276.75	272.85		444.77
	1100	441.65	486.01	271.25	269.52		439.93
M2	900	450.96	480.16	281.68	276.70		447.64
	1000	446.49	470.28	276.75	272.85		443.15
	1100	441.65	459.06	271.25	269.52		438.30
Mo ₁	900	450.96	499.62	281.68	276.70	299.92	449.64
	1000	446.49	494.53	276.75	272.85	301.04	445.17
	1100	441.65	489.90	271.25	269.52	299.09	440.35
Mo ₂	900	450.96	500.00	281.68	276.70	299.92	449.58
	1000	446.49	495.49	276.75	272.85	301.04	445.12
	1100	441.65	490.76	271.25	269.52	299.09	440.30
Mo ₃	900	450.96	498.16	281.68	276.70	299.92	449.55
	1000	446.49	493.32	276.75	272.85	301.04	445.08
	1100	441.65	489.18	271.25	269.52	299.09	440.27

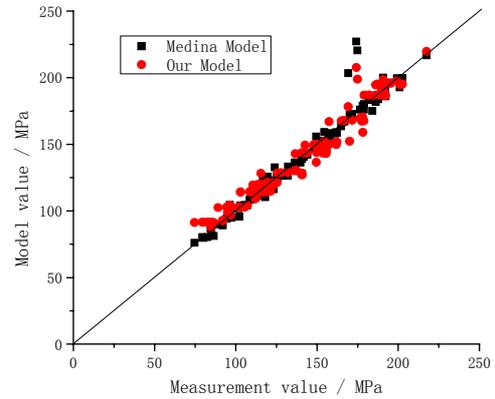


Figure 2 The peak stress model results of low-alloy steel

Conclusions

1. A method from the thermal expansion data to calculate the austenite lattice constant at high temperature can be used to calculate the valence electron parameters of the austenite at high temperature, and then their statistical value can be calculated further;
2. In accordance with rank 11 of Fe B-type hybrid in austenite the every unit cell binding energies were calculated, and the total binding energy of the austenitic at high temperature were calculated with the mole fraction of elements in the low alloy steel;
3. The peak stress models of the austenitic at high temperature were gained based on the total binding energy, and the statistical results show that our model is more accurate than Medina model.

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